Bootstrapped gross error detection for efficient and fault-tolerant real-time optimization

American Control Conference: July 10th, 2024

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ACC 2024

Outline

1. Introduction and motivation for online economic optimization
2. Two-step real time optimization (RTO)
    a. Theory
    b. Drawbacks and motivation
3. Bootstrapped gross error detection (GED) for RTO
    a. Formulations
    b. Bootstrapping
    c. Fault-identification
    d. CSTR case study

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Online economic optimization

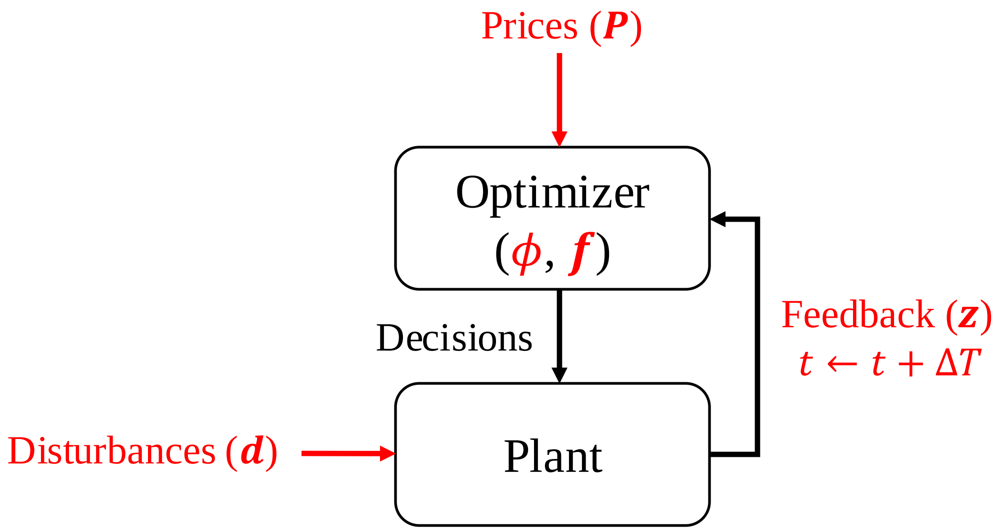
Why?

- Disturbances ($\boldsymbol{d}$)
- Changing economics ($\boldsymbol{P}$)
- Competitiveness
- Sustainability

How?

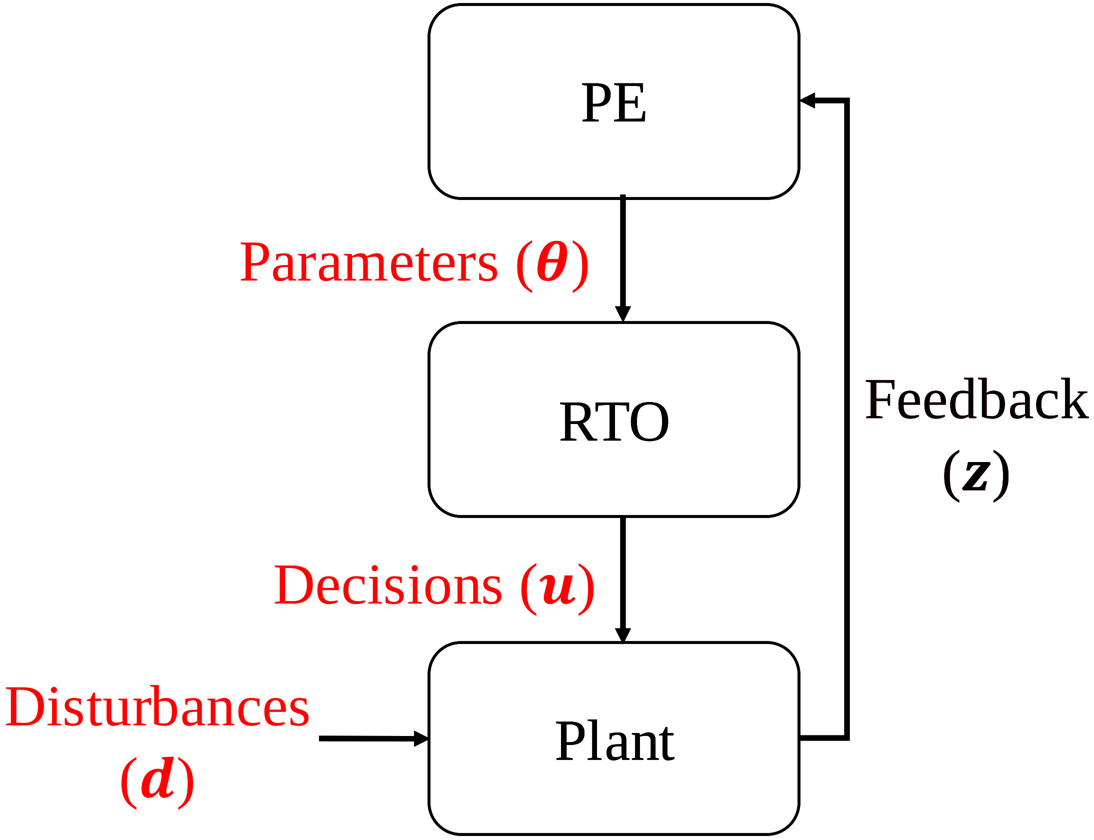
- Economic model (ϕ)
- Process model ($\boldsymbol{f}$)
- Sensor measurements ($\boldsymbol{z}$)

Uncertainty



The two-step real-time optimization[1]

- A real-time optimizer (RTO) provides economically optimal decisions ($\boldsymbol{u}$) to the plant
- The plant is subject to disturbances ($\boldsymbol{d}$) and provides feedback ($\boldsymbol{z}$)
- A parameter estimation (PE) problem provides the RTO with updated uncertainties ($\boldsymbol{\theta}$) at every execution



[1] M.L. Darby, M. Nikolaou, J. Jones, D. Nicholson. *J. Process Control*, vol. 21, no. 6, pp. 874–884. 2011.

Drawbacks of two-step RTO

- Instrumentation faults can lead to measurement bias i.e., systematic error
- Measurement error can propagate to the estimated parameters
- The parameter errors can result in economic suboptimalities and constraint violations

Goals for GED-RTO

- Pose parameter-driven GED method that is easily retrofitted[2,3,4] into existing RTO systems
- Leverage computational resources to achieve GED without requiring additional RTO steps[5]

[2] S.A. Bhat, D.N. Saraf. *Ind. Eng. Chem. Res.*, vol. 43, no. 15, pp. 4323–4336. 2004.
[3] D.B. Özyurt, R.W. Pike. *Comput. Chem. Eng.*, vol. 28, no. 3, pp. 381–402. 2004.
[4] I. Kim, M.S. Kang, S. Park, T.F. Edgar. *Comput. Chem. Eng.*, vol. 21, no. 7, pp. 775–782. 1997.
[5] G.D. Patrón, L. Ricardez-Sandoval. *Ind. Eng. Chem. Res.*, vol. 61, no. 45, pp. 16780–16798. 2022.

Two-step RTO formulations[1]

$$\min_{\boldsymbol{u}} \phi(\boldsymbol{u}, \widehat{\boldsymbol{x}},)$$
$$s.t.$$
$$\boldsymbol{f}\left(\boldsymbol{d}, \boldsymbol{u}, \widehat{\boldsymbol{x}}, \widehat{\boldsymbol{\theta}}\right) = \mathbf{0}$$
$$\boldsymbol{g}(\boldsymbol{d}, \boldsymbol{u}, \widehat{\boldsymbol{x}}) \leq \mathbf{0}$$
$$\boldsymbol{u}_{\boldsymbol{min}} \leq \boldsymbol{u} \leq \boldsymbol{u}_{\boldsymbol{max}}$$
$$\boldsymbol{u} \in \mathbb{R}^{n_u}, \boldsymbol{d} \in \mathbb{R}^{n_d}, \widehat{\boldsymbol{x}} \in \mathbb{R}^{n_x}$$

$$\min_{\widehat{\boldsymbol{\theta}}} \|\widehat{\boldsymbol{z}} - \overline{\boldsymbol{z}}\|_{\boldsymbol{Q_z}^{-1}}{}^2$$
$$s.t.$$
$$\boldsymbol{f}(\boldsymbol{d}, \boldsymbol{u}, \widehat{\boldsymbol{x}}, \widehat{\boldsymbol{\theta}}) = \mathbf{0}$$
$$\boldsymbol{h}(\widehat{\boldsymbol{x}}) = \widehat{\boldsymbol{z}}$$
$$\boldsymbol{\theta}_{\boldsymbol{min}} \leq \widehat{\boldsymbol{\theta}} \leq \boldsymbol{\theta}_{\boldsymbol{max}}$$
$$\boldsymbol{z} \in \mathbb{R}^{n_z}, \ \widehat{\boldsymbol{\theta}} \in \mathbb{R}^{n_\theta}$$

- Economic function (ϕ) solved subject to steady-state model ($\boldsymbol{f}$)
- ϕ dependence on state and input variables ($\boldsymbol{u}, \widehat{\boldsymbol{x}}$)
- Model subject to parameters ($\boldsymbol{\theta}$)

- Least-squares minimization of measurement predictions ($\widehat{\boldsymbol{z}}$) and averaged measurements ($\overline{\boldsymbol{z}}$)
- Uses inverse covariance matrix ($\boldsymbol{Q_z}^{-1}$) for weighting

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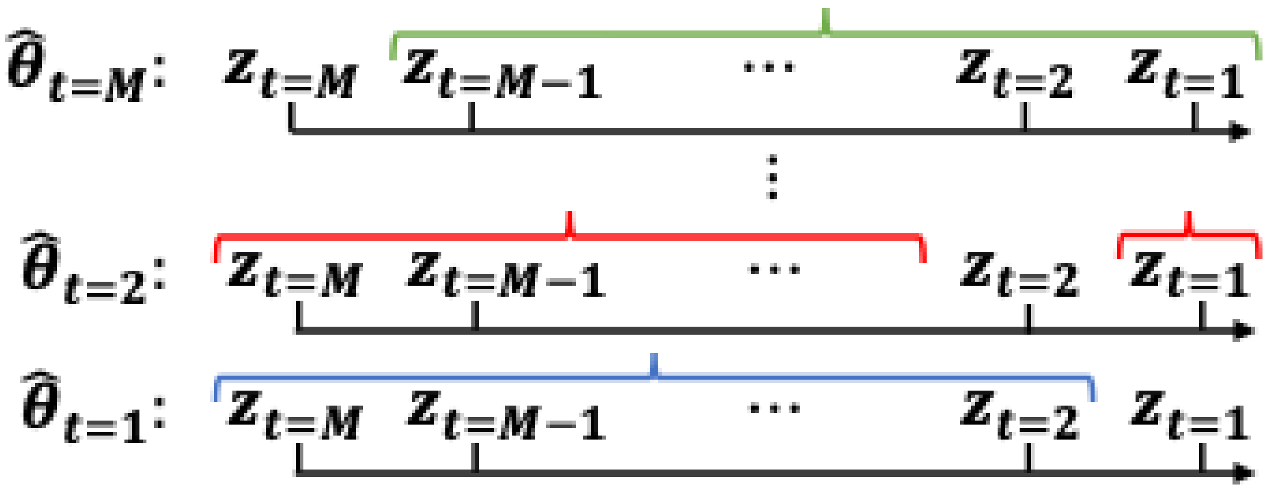
[1] M.L. Darby, M. Nikolaou, J. Jones, D. Nicholson. *J. Process Control*, vol. 21, no. 6, pp. 874–884. 2011.

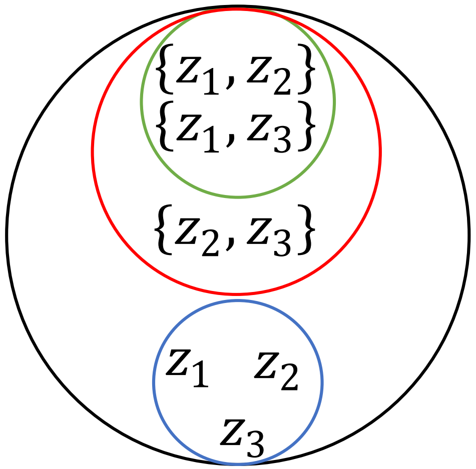
Parameter bootstrapping[5]

- Build estimated parameter sample through bootstrapping
- Re-sample the measurement sample $\{\mathbf{z}_{t=i}\}_{i=1}^{M}$ using $M-1$ measurements
- Each measurement subsample is used to generate a least-squares parameter sample $\{\hat{\boldsymbol{\theta}}_{t=i}\}_{i=1}^{M}$



[5] G.D. Patrón, L. Ricardez-Sandoval. *Ind. Eng. Chem. Res.*, vol. 61, no. 45, pp. 16780–16798. 2022.

Measurement sets



$$\mathcal{M} = \{z_1, z_2, z_3\}$$

$$\mathcal{P}(\mathcal{M}) = \{\{\ \}, \{z_1\}, \{z_2\}, \{z_3\}, \{z_1, z_2\}, \{z_1, z_3\}, \{z_2, z_3\}, \{z_1, z_2, z_3\}\}$$

$$\mathcal{S} = \mathcal{P}_2\left(\mathcal{M}\right) = \{\{z_1, z_2\}, \{z_1, z_3\}, \{z_2, z_3\}\}$$

$$\mathcal{S}_{z_1} = \{\{z_1, z_2\}, \{z_1, z_3\}\}$$

- $\mathcal{M}$ is measurement set
- $\mathcal{P}(\mathcal{M})$ is the power set of measurements
- $\mathcal{S} = \mathcal{P}_K\left(\mathcal{M}\right)$ is the cardinality K subset of the power set
- $\mathcal{S}_j = \{\mathcal{S} | j \in \mathcal{S}\}$ is the subset of $\mathcal{S}$ containing measurement j

Multi-parameter t-test

- Hypothesis test:

$$H_0 : \overline{\boldsymbol{\theta}} = \overline{\boldsymbol{\theta}}_{\boldsymbol{i}}$$

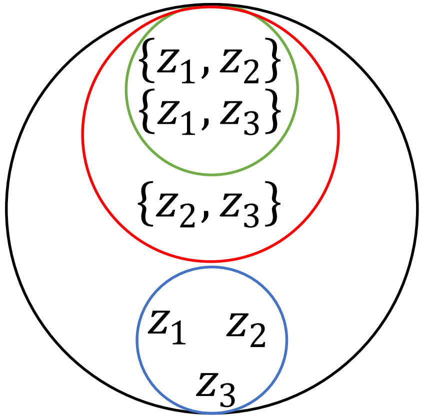
$$H_1 : \overline{\boldsymbol{\theta}} \neq \overline{\boldsymbol{\theta}}_{\boldsymbol{i}}$$

- Rejection criteria:

$$\|-\boldsymbol{P}_{\boldsymbol{i}}\|_\infty > -\alpha \ \forall i \in \mathcal{S}_j$$

- If multiple faults, sensor with largest probability of being faulty is:

$$j = argmax\left\{\|-\boldsymbol{P}_{\boldsymbol{i}}\|_\infty | \forall i \in \mathcal{S}_j | \forall j \in \mathcal{M}\right\}$$



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Parameter-driven GED approach for RTO

1. Collect an M-length steady-state sample of $\mathcal{M}$:

$$\{\boldsymbol{z}\}_{t=1}^{M}$$

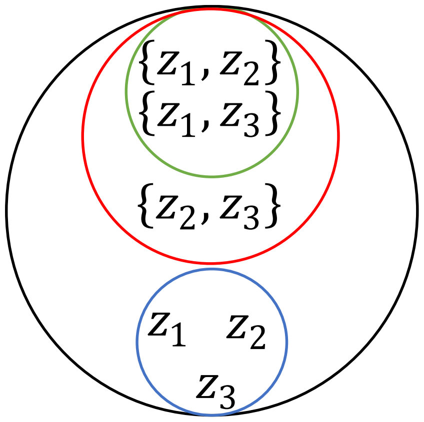
2. Construct partial measurement vectors:

$$\boldsymbol{\zeta_i} \forall i \in \mathcal{S}$$

3. Compute parameter-estimate samples:

$$\{\boldsymbol{\theta}_i\}_{t=1}^{M} \forall i \in \mathcal{S}$$

4. Perform t-test. Do all measurements lead to statistically equivalent estimates?
   a. Yes: go to 5
   b. No: remove measurement with highest probability of being erroneous and go to 2
5. Execute RTO with gross error omitted and provide decision to plant



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Computational complexity

- Worst-case complexity is for scenario when measurements are reduced to $n_{z,min}$
- A combinatorial number of potential measurement subsets of $n_{z,min}$ cardinality given a set of n_z measurements:

$$n_K\left(n_z, n_{z,min}\right) = \frac{n_z!}{n_{z,min}!\left(n_z - n_{z,min}\right)!}$$

- Accordingly, the bootstrapping procedure requires the following number of PE problems to be solved pessimistically:

$$n_{PE} = n_K \times M$$

CSTR case study[6]

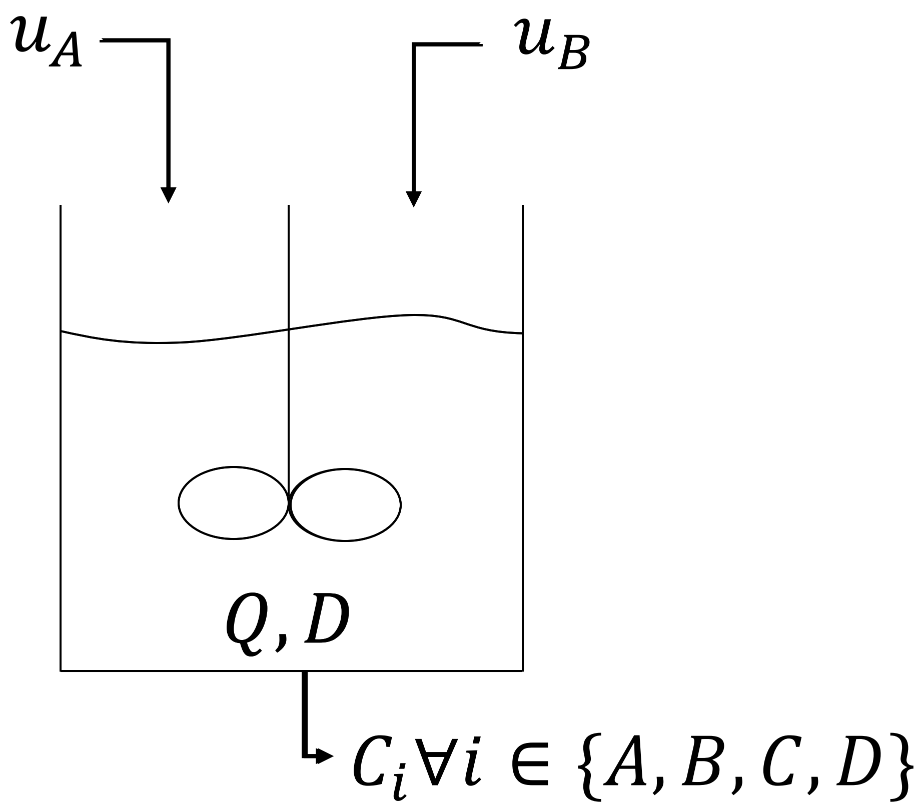
- Maximize productivity in C while minimizing input
- Impose maximum heat generation (Q) and selectivity (D)

$$\max_{\boldsymbol{u}} \phi \coloneqq \frac{{C_C}^2 (u_A + u_B)^2}{u_A C_{A,in}} - w({u_A}^2 + {u_B}^2)$$

$$\boldsymbol{f}(\boldsymbol{u}, \hat{\boldsymbol{x}}, \hat{\boldsymbol{\theta}}) = \boldsymbol{0}$$

$$g_j \leq 0 \; \forall j \in \{Q, D\}$$

$$0 \leq u_A, u_B \leq u_{max}$$



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[6] G. François, D. Bonvin. Ind. Eng. Chem. Res., vol. 53, no. 13, pp. 5148–5150. 2013.

CSTR case study

- Reaction kinetics constants are the estimated parameters:

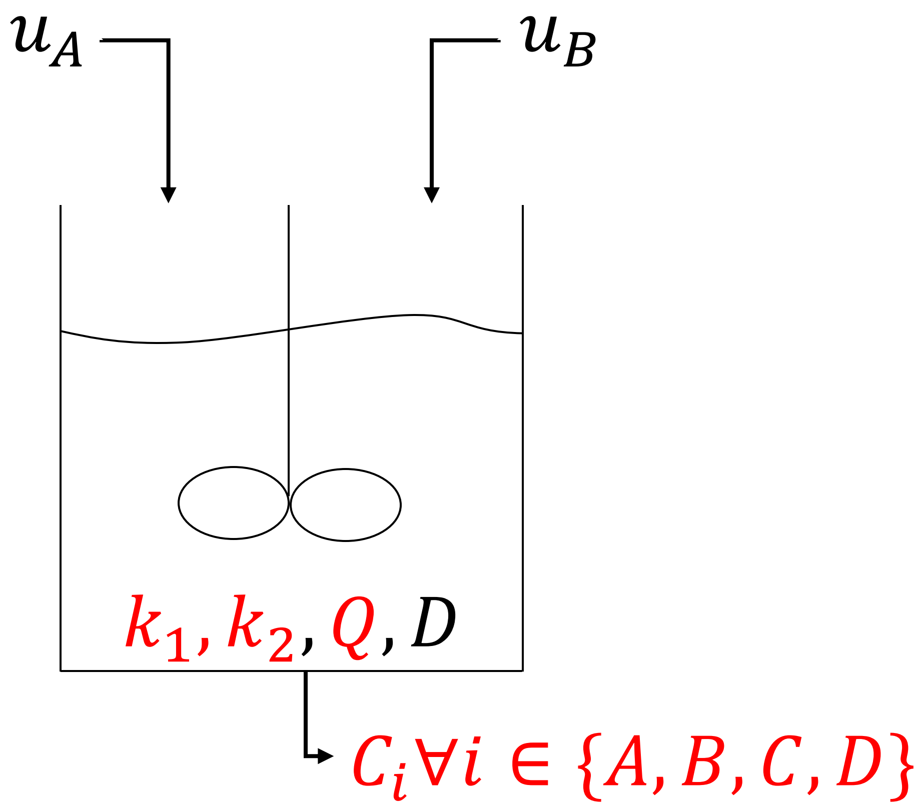
$$\boldsymbol{\theta} = [k_1 \quad k_2]^T$$

- Measurements are comprised of composition and heat generation:

$$\boldsymbol{z} = [C_A \quad C_B \quad C_C \quad C_D \quad Q]^T$$

- Faults inserted into random sensors from uniform distribution:

$$\boldsymbol{f} \sim U[-0.3\boldsymbol{z_{nom}}, 0.3\boldsymbol{z_{nom}}]$$



CSTR case study

- Single and double fault case studied
- RTO vs RTO+GED compared on:
  - Parameter error (e_{k_1}, e_{k_2})
    - Lower error with GED
  - Cumulative constraint violation (SAV)
    - Better satisfaction with GED
  - Process profit ($\bar{\phi}$)
    - Same cost
  - # of correctly detected faults

	Single fault case		Double fault case	
Metric	**RTO**	**RTO+GED**	**RTO**	**RTO+GED**
$e_{k_1}(\%)$	8.75	1.55	8.11	1.38
$e_{k_2}(\%)$	9.60	4.90	4.57	1.24
$SAV(kcal/min)$	46.97	3.91	26.83	2.72
$\bar{\phi}$	15.27	15.27	15.41	15.41
# of faults inserted	–	100	–	200
# of faults correctly detected	–	88	–	160

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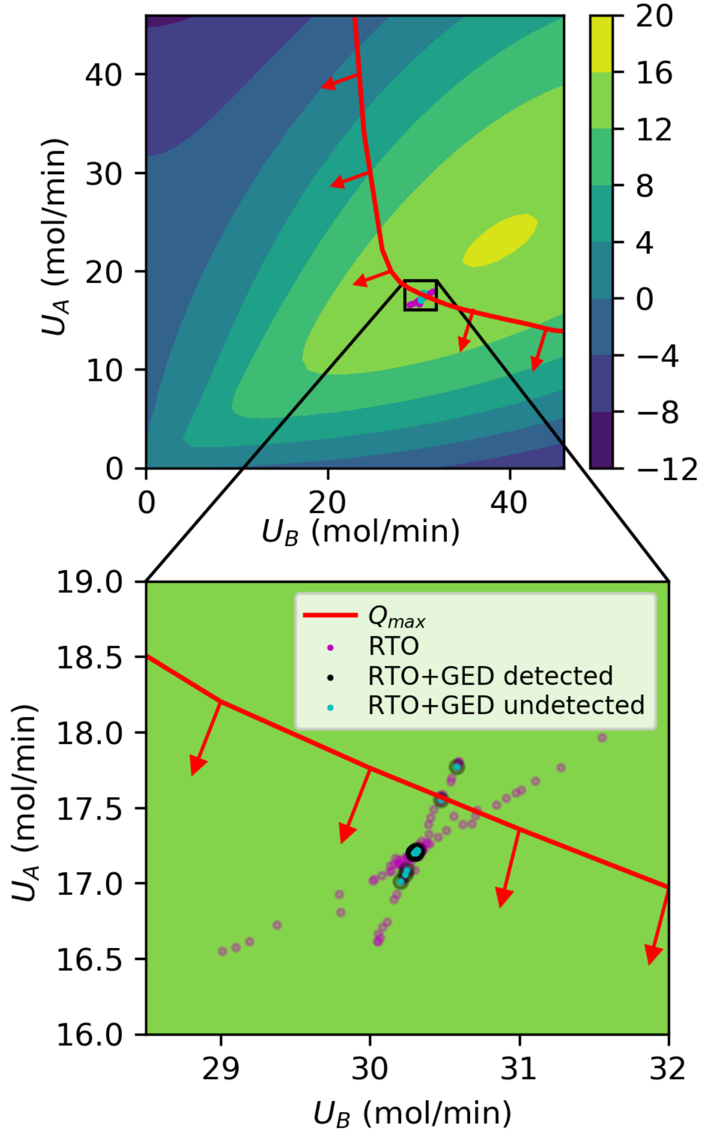

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Conclusions

- A novel bootstrapped GED approach was proposed:
  - Easily retrofitted into existing RTO
  - Leverages modern computational resources
- Effect of gross errors abated in CSTR:
  - High percentage of faulty sensors found
  - Better constraint satisfaction (i.e., safer)

Future work

- Lower computational complexity (important for large systems)

Acknowledgements

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References

[1] M.L. Darby, M. Nikolaou, J. Jones, D. Nicholson, "RTO: An overview and assessment of current practice," *J. Process Control*, vol. 21, no. 6, pp. 874–884, Jul. 2011.

[2] S.A. Bhat, D.N. Saraf, "Steady-State Identification, Gross Error Detection, and Data Reconciliation for Industrial Process Units," *Ind. Eng. Chem. Res.*, vol. 43, no. 15, pp. 4323–4336, Jun. 2004.

[3] D.B. Özyurt, R.W. Pike, "Theory and practice of simultaneous data reconciliation and gross error detection for chemical processes," *Comput. Chem. Eng.*, vol. 28, no. 3, pp. 381–402, Mar. 2004.

[4] I. Kim, M.S. Kang, S. Park, T.F. Edgar, "Robust data reconciliation and gross error detection: The modified MIMT using NLP," *Comput. Chem. Eng.*, vol. 21, no. 7, pp. 775–782, Mar. 1997.

[5] G.D. Patrón, L. Ricardez-Sandoval, "Low-Variance Parameter Estimation Approach for Real-Time Optimization of Noisy Process Systems," *Ind. Eng. Chem. Res.*, vol. 61, no. 45, pp. 16780–16798, Nov. 2022.

[6] G. François, D. Bonvin, "Use of Transient Measurements for the Optimization of Steady-State Performance via Modifier Adaptation," *Ind. Eng. Chem. Res.*, vol. 53, no. 13, pp. 5148–5150, Sept. 2013.